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# ***JPRS Report—***

## **Science & Technology**

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***USSR: Chemistry***

# Science & Technology

## Chemistry

JPRS-UCH-88-009

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**Standard Samples for Control of Chemical Composition of Ferrous Metallurgy Materials by Chemical and Spectral Analytical Methods**  
18410195a Moscow ZHURNAL ANALITICHESKOY KHMII in Russian Vol 42, No 11, Nov 87 (manuscript received 2 Apr 86) pp 1973-1976

[Article by V.V. Stepin, V.I. Ustinova, N.D. Fedorova, N.V. Stashchikova, V.I. Kurbatova, and V.A. Kozmin, Institute of Standard Reference Samples, Ferrous Metallurgy Central Scientific Research Institute imeni I.P. Bardin, Sverdlovsk]

[Abstract] The Institute of Standard Reference Samples of the Ferrous Metallurgy Central Scientific Research Institute has released a number of standard samples (SO) of steels, nickel alloys, cast iron, and master alloys containing rare earth elements. The total amount, expressed as a percentage, of each element has been established through interlaboratory collaboration. The values for certified specifications and random errors are listed in four tables. References 4 (Russian).

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**Annual Session of Siberian Department of Learned Council of USSR Academy of Sciences on Analytical Chemistry and Novosibirsk Seminar on Analytical Chemistry**  
18410195b Moscow ZHURNAL ANALITICHESKOY KHMII in Russian Vol 42, No 11, Nov 87 pp 2101-2103

[Article by M.M. Goldshteyn]

[Abstract] The annual session of the Siberian Department of the USSR Academy of Sciences Learned Council on Analytical Chemistry and the Novosibirsk Seminar on Analytical Chemistry on the topic "Automation, Robotization, and Computerization of Analysis" were held in Novosibirsk from 2 to 4 December 1986. Over 70 specialists took part in the proceedings. Participants in the session approved the results of the department's scientific and organizational work for 1986 and noted its growing role in coordinating research. Reports by the Kemerovsk, Tomsk, and Tyumen regional commissions were heard, and 18 reports were given on the development and utilization of laboratory robots, automated systems, and computer technology, as well as the results of research directed toward broadening the use of mathematical methods and automating analysis.

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**Reliability of Photometric Methods in Determining Harmful Impurities in Workplace Air**  
18410265b Moscow GIGIYENA TRUDA I PROFESSIONALNYYE ZABOLEVANIYA in Russian No 2, Feb 88 (manuscript received 10 Nov 85) pp 57-60

[Article by A.A. Belyakov and L.V. Melnikova, Institute of Labor Hygiene and Occupational Diseases, Gorkiy]

[Abstract] Many recommended photometric methods for determining harmful impurities in air have never been evaluated for their reliability or been certified. This article presents a simple method for evaluating the reliability of methods for determining the vapors of liquid and solid organic compounds and describes a dosing unit that utilizes the gas jet dilution method. The dosing installation consists of two parts. A constant laminar flow of the initial gas mixture at 0.1-0.35 l/min is created in the first part, while the gas mixture is diluted with pure air at 0.5-4 l/min in the combined system. The results obtained by the physical and chemical methods were compared to confirm the estimates of the reliability of the determination of dimethylpiperazine, aniline, chloroform, and alkylmethacrylate. The agreement between the two methods was found to be satisfactory. Figures 3, references 20: 19 Russian, 1 Western.

06508

**EPR Spectrometer for Operation in Weak Magnetic Fields**

18410265a Novosibirsk IZVESTIYA SIBIRSKOGO OTDELENIYA AKADEMII NAUK SSSR: SERIYA KHMICHESKIYE NAUKI in Russian No 1, Jan-Feb 88 (manuscript received 11 Sep 86) pp 121-125

[Article by A.V. Koptyug, Institute of Chemical Kinetics and Combustion, Siberian Department, USSR Academy of Sciences, Novosibirsk]

[Abstract] Weak-field EPR studies are of interest as a possible method of coal prospecting. Detailed EPR spectral studies of various geological specimens in weak fields approximating the terrestrial magnetic field are therefore needed. EPR spectra of specimens with a high water content are needed in biology and medicine to study the feasibility of their in vivo use. Specimens with significant dielectric permeability or high conductivity must also be studied in other areas, although work with such specimens in the microwave band is quite difficult due to the frequency detuning of the resonator as a specimen is inserted. There are no commercially manufactured weak-field EPR spectrometers. This article describes the development of such a device, capable of recording EPR spectra from specimens as large as several cubic centimeters in magnetic fields of one to a few hundred Gauss, with a sensitivity equal to that of existing instruments. The device developed has 10 sensors operating at fixed frequencies in the 15 to 300 MHz band with a sensitivity of no less than  $5 \times 10^{14}$  spins per

specimen and a resolution of at least 0.1 Gauss/s. The sensors are LC circuits with concentrated inductance and capacitance that are matched with a 50 Ohm line through a capacitance coil or resonator with a spiral internal wire and operate with the natural distributed capacitance of the coil. A functional diagram of the device is presented. It is distinguished by its broad band of operating frequencies and ability to shift from one

sensor frequency to another without changing the design of the instrument due to the use of wideband HF amplifiers, a bandwidth of up to 300 MHz, a wideband synchronous HF detector, and wideband hybrid loops with a directed branching circuit. Figures 2, references 13: 3 Russian, 10 Western.

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**Technology, Production Development, and Properties of Domestic Ultrafiltration and Reverse-Osmosis Membranes**

18410216b Moscow ZHURNAL VSESOYUZNOGO KHIMICHESKOGO OBSHCHESTVA IM. D.I. MENDELEYEVA in Russian Vol 32, No 6, Nov-Dec 87 pp 627-633

[Article by V.P. Dubyaga and Ye.Ye. Katalevskiy, "Polimersintez" Scientific Production Organization]

[Abstract] Membrane technology is among the avant garde directions of modern science and technology, with annual sales worldwide estimated at close to 1 billion dollars and with a growth rate estimated between 7-10 and 20-30%. Membrane separation processes based on reverse-osmosis ultrafiltration membranes differ from the usual slime filtration process in that in reverse-osmosis ultrafiltration, the substances dispersed in the water are held in the membrane's surface layer and are continually washed away by the tangential flow of the liquid that is being separated. This makes it possible to conduct a filtration process for an extended period before having to replace the filter material. Reverse osmosis is currently being used to desalinate more than 2 million cubic meters of salt and sea water daily, thereby making it suitable for domestic, industrial, and other purposes. The process is useful in other areas as well, including environmental protection (cleaning industrial wastewater) and the dairy and food industries (concentrating sucrose, lactose, and fruit juices). Estimates place the profit derived from producing 1 ton of lactose at 670.0 rubles when the traditional method is used versus 710.0 rubles when the reverse-osmosis technique is used. The technique is not without its limitations, however. Progress has been made with respect to developing and producing highly selective membranes with low hydraulic resistance and a high degree of permeability. Cellulose acetate has been considered a good material for reverse-osmosis and ultrafiltration membranes for a quite a while. Other materials that show promise include aromatic polyamides, polybenzimidazoles, aromatic polysulfones, polyamide hydrazides, and polypiperazine amides. Membrane technology has been specified as one of the top-priority directions in scientific-technical progress. It has paved the way for the creation of resource-saving and waste-free production processes. For this reason, a wide-scale program of developing and organizing the production of membranes, membrane units, and filter elements has been undertaken in the USSR. Figure 1; references 17: 11 Russian, 6 Western.

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**Urgent Problems in Modern Membrane Technology**

18410216a Moscow ZHURNAL VSESOYUZNOGO KHIMICHESKOGO OBSHCHESTVA IM. D.I. MENDELEYEVA in Russian Vol 32, No 6, Nov-Dec 87 pp 603-605

[Article by Professor A.S. Chegolya, Ministry of the Chemical Industry]

[Abstract] The success of efforts to develop new-generation membranes and to implement new highly effective membrane processes of separating liquid and gaseous mixtures will be determined largely by the depth of understanding of the functional principles of membrane systems and by the development of physicochemical concepts related to the transfer mechanisms of ions and molecules through synthetic membranes. A rather diverse array of membrane separation mechanisms are currently being implemented. Reverse-osmosis polymer membranes for water desalination are being developed. The Rodnik electrodialysis unit, which was developed by the Plastmassy Scientific Production Association [NPO], makes it possible to obtain 2 m<sup>3</sup>/h drinking water from salt water. Production of second-generation gas-separating membranes from polysulfamide substrates and modern duct components made of ultrafiltration hollow fibers has been organized at the Kusk Chemical Plant. A number of institutes and NPOs, including the Joint Nuclear Research Institute, Polimersintez NPO, and Leningrad Chemical Fiber Scientific Research Institute [LenNIIkhimvolokno], were involved in the creation and industrial implementation of modules and units based on hollow fibers. Some promising areas for future development of membrane technology include membrane catalysts, bioreactors, and extraction of useful components from industrial wastewater and various gas streams. References 19: 5 Russian, 14 Western.

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**Nuclear Filters: New Class of Microfiltration Membranes for Precision Separation of Colloid Solutions**

18410216c Moscow ZHURNAL VSESOYUZNOGO KHIMICHESKOGO OBSHCHESTVA IM. D.I. MENDELEYEVA in Russian Vol 32, No 6, Nov-Dec 87 pp 641-647

[Article by B.V. Mchedlishvili, Institute of Crystallography imeni A.V. Shubnikov, USSR Academy of Sciences, and Academician G.N. Flerov, Joint Institute of Nuclear Research, Dubna]

[Abstract] Microfiltration, a membrane process of separating fine suspensions and colloid solutions, is one of the most widely used production techniques based on using porous baffles. Nuclear filters constitute a new class of porous membranes. The effect of a rapid increase in the selectivity of track etching, coupled with an increase in the atomic number of the ion, is one of the factors that makes it possible to control the pore shape of nuclear filters as early as the stage in which the source film is irradiated with highly charged ions. The degree of etching selectivity, and thus the por. shape, can be controlled by varying the temperature and concentration of the etching agent. Nuclear filters have been approved for use in the pharmaceutical industry, medicine, and chemical and

food production. Processes of the membrane separation of colloid solutions proceed successfully if there is no adsorption in the membranes' active centers, and nuclear filters allow for all types of heat sterilization except those above 200° C, at which point their properties change. Productivity is one of the most important parameters of membrane separation. The productivity of track membranes virtually coincides with that of mesh membranes, or even surpasses it. The separating capability of microfiltration processes is largely determined by the value of the ratio of the

dimensions of the particles being filtered to the membrane pores,  $\lambda d/D$ . In recent years, track filters, above all nuclear filters, have found increasingly more diverse uses in such areas as analyzing environmental pollution, cleaning liquids and gases for use in microelectronics, stabilizing beverages, and discovering and studying the dimensions and form of cells and viruses. Figures 11; references 44: 30 Russian, 14 Western.

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**Structural Changes During Nongaseous Combustion in Heterogeneous Systems Containing Molten Metallic Reagent**

18410210b Moscow *DOKLADY AKADEMII NAUK SSSR* in Russian Vol 298, No 2, Jan 88 (manuscript received 4 Aug 87) pp 414-417

[Article by B.M. Khusid and A.G. Merzhanov, presented by USSR Academy of Sciences Academician Yu.A. Buslayev, Institute of Chemical Physics, Chernogolovka Branch, USSR Academy of Sciences, Moscow Oblast]

[Abstract] The characteristics and mechanism of nongaseous combustion of metal-nonmetal systems have been described in works on self-propagating high-temperature synthesis. Problems related to the nature and speed of combustion front propagation, the thermal structure of a combustion front, and the composition and morphology of end products have also been studied. The most detailed information available is that about titanium-based systems. However, the mechanism and kinetics of structure formation of the end products, which are components of the subject area of structural macrokinetics, have hardly been studied. In a previous part of this work, experimental data were presented on the structural changes in a mixture of titanium, carbon, and boron powders. The present part presents the results of an analysis of the dynamics of the structural changes that take place during the combustion of a titanium-carbon mixture. One distinctive feature of the structural macrokinetics of nongaseous combustion in this type of system is the melting of the metal and the associated effects of capillary flow (or capillary penetration). The analysis is based on the characteristic times for a wide range of various physicochemical and thermal processes taking place in a combustion wave. Analogous processes such as melting and crystallization, changes in chemical and phase composition, and dispersion, which take place under the traditionally lower temperature conditions of furnace synthesis, occur three to six orders of magnitude more slowly than during combustion. Due to the great difference in activation energies of the individual stages of these processes, those factors that determine the structural macrokinetics inside the synthesis wave and in traditional technologies (especially with materials approaching those used in powder metallurgy) are essentially different. These differences are mainly due to the leading role of chemical changes associated with combustion. Analysis of the structural macrokinetics of combustion of the systems showed that three stages exist. During the first stage, lasting  $10^{-2}$  to  $10^{-3}$  seconds, the primary reaction product is formed. It commences within the heating zone preceding the combustion front. The governing processes are titanium particle melting and penetration of the melt into the surrounding layer of carbon particles, thereby controlling the kinetics of carbide formation. The end product is formed in the second stage, lasting  $10^{-1}$  to  $10^{-2}$  seconds. The main processes consist of an increase in carbon content in the carbide and a drop in the supersaturation of the melt. During the

last stage, lasting 1 to 5 seconds, the carbide particles coalesce at approximately 10 microns per second. References 15: 13 Russian, 2 Western.

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**Effect of Physicochemical Properties of Gas and Liquid on Parameters and Conditions for Existence of Detonation Waves in Liquid-Gas Bubble Systems**

18410215b Novosibirsk *FIZIKA GORENIYA I VZRYVA* in Russian No 6, Nov-Dec 87 (manuscript received 4 Aug 86) pp 76-84

[Article by A.V. Pinayev and A.I. Sychev, Novosibirsk]

[Abstract] The present work was conducted to determine the conditions needed for the existence of a detonation wave and to clarify the effects of the properties of components of the system (composition of the gas mixture, type of liquid and its viscosity) on the limits of detonation propagation. Experiments were carried out in a vertical shock tube (35 mm in diameter, 4 m long) filled with a liquid having uniformly distributed gas bubbles (2 to 4 mm in diameter). Detonation parameters were recorded with a piezoelectric pressure sensor, and the incandescence of the gas-liquid system was measured with a photoelectric amplifier. The two systems studied were a water-glycerin mixture containing bubbles of mixtures of oxygen, ethane, propane, and air with acetylene, and a VM-3 vacuum oil, containing oxygen-nitrogen bubbles. The lower and upper concentration limits of detonation were determined for both gas components and gas phase content. The viscosity of the liquid component of the mixture was observed to have a significant effect on the conditions for the existence and parameters of a detonation. This is evidently due to the relationship of viscosity to such processes as instability of bubble surfaces, heat losses, gas temperature prior to ignition, and ignition delay. Figures 5; references 20: 14 Russian, 6 Western.

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**Turbulent Combustion of Hydrogen in Near-Wall Jet Escaping into Adjacent Air Stream**

18410215a Novosibirsk *FIZIKA GORENIYA I VZRYVA* in Russian No 6, Nov-Dec 87 (manuscript received 2 Mar 87) pp 3-9

[Article by V.G. Gromov, O.B. Larin, and V.A. Levin, Moscow]

[Abstract] A numerical analysis was made of the ignition and combustion of low-temperature hydrogen in a turbulent near-wall stream escaping through a flat slit into an adjacent ultrasonic hot air stream. The multilayer algebraic model used in the analysis was based on the hypothetical length of the mixing route and Jones and Launder's differential two-parameter  $k - \epsilon$  model. It is

demonstrated that the proposed modification of the so-called nonmixing model provides better agreement with experimental data. Figures 6; references 17: 8 Russian, 9 Western.

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**Estimating Pressure within Low-Velocity Detonation Wave of Compressed PETN**

18410215c Novosibirsk *FIZIKA GORENIYA I VZRYVA* in Russian No 6, Nov-Dec 87 (manuscript received 20 Dec 83) pp 84-86

[Article by V.F. Martynyuk, A.A. Sulimov, M.K. Sukyan, and A.V. Obmenin, Moscow]

[Abstract] Stationary low-velocity detonation in compressed explosives has only been observed for charges enclosed within a shell. In this case, the steady state of the process was judged by the lack of change in detonation velocity and the final deformation of the internal channel of the shell at the conclusion of the process. Reliable data on the pressure profile of low-velocity detonation in a metal shell are essentially lacking, mainly due to the difficulties entailed in using traditional methods for measuring pressure under these conditions. In the present work, a study was made of the dynamics of deformation of a steel shell during low-velocity detonation propagation in compressed PETN (pentaerythritol tetranitrate) having a density of 1.73 g/cm<sup>3</sup>. The charge was loaded into a steel shell having internal and external diameters of 10 and 16 mm, respectively. It was demonstrated that the process is stationary and propagates at a velocity of 2,300 to 2,600 m/s, depending on the particle size of the product. The pressure in a low-velocity detonation wave was estimated from the resulting change in the external shell diameter by using the thin-shell formula. Figures 2; references 7: 6 Russian, 1 Western.

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**Effect of Compressibility of Additive Material on Detonation Velocity of Mixed Charges**

18410215d Novosibirsk *FIZIKA GORENIYA I VZRYVA* in Russian No 6, Nov-Dec 87 (manuscript received 6 Feb 86) pp 86-89

[Article by I.M. Voskoboinikov, M.F. Gogulya, and G.V. Dimza, Moscow]

[Abstract] The detonation parameters of explosives decrease when inert substances are added to the charge as a result of the compression, dispersal, and heating of the additive particles. The characteristic times for the conclusion of these processes vary and increase with number. By selecting the particle size of the charge

components, it is possible to create a situation during the decomposition time of an explosive in a detonation wave wherein the additive particles will be compressed and entrained within the stream of the explosion products but will remain essentially unheated. In this case, the decrease in detonation parameters is determined solely by the compressibility of the additive material, and information on any pressure-dependent changes therein may be obtained by analyzing the decrease in the detonation parameters of a single explosive of varying density or of charges of various substances having similar densities. In the present work, detonation velocities were determined for mixed charges of trotyl-, hexogen-, and octogen-containing additives of sodium and potassium chloride, boron nitride, benzene, hexane, and a solution of carbon tetrachloride and hexane having a density equal to that of benzene. Analysis of the data showed that the behavior of the additives under shock load results in a supplemental decrease in the detonation velocity of a mixed charge. Tables 1; references: 6 Russian, 1 Western.

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**Nonadiabatic Heterogeneous Reaction Wave Propagation Modes through Metal Fiber**

18410259b Moscow *DOKLADY AKADEMII NAUK SSSR* in Russian Vol 299, No 2, Mar 88 (manuscript received 1 Jun 87) pp 399-405

[Article by V.I. Lyubchenko and G.N. Marchenko; presented by Academician V.I. Goldanskiy]

[Abstract] The study examined the possibility of the occurrence of reaction diffusion when a metal filament heated by an electric current reacts with the surrounding medium. A layer of condensed product having a lesser specific electrical conductivity than the source metal is formed in the process. It was hypothesized that the heterogeneous reaction is thermally neutral, that the electrical resistance of the metal filament is not temperature dependent, and that the coefficient of the reagent's diffusion in the layer is an exponential function of the temperature. A mathematical model of the process was formulated. The model assumed an equal activation energy in the electrical resistances of the metal and the reaction product and a linear distribution of the concentration of the diffusing reagent in the reaction layer, and it made an allowance for the nonisothermal nature of the reaction diffusion process, a joulean heat liberation in the filament, and heat transfer from the surface of the filament to the surrounding medium. The model was used to calculate the linear velocity of the thermal wave, the temperature and thickness of the layer of reaction products, and the propagation rate of the reaction wave. References 8: Russian.

06508

**Electrochemical System for Removing Carbon Dioxide from Atmosphere and Regenerating Oxygen with Carbonate Electrolyte**

18410203a Moscow *ELEKTROKHIMIYA* in Russian  
(manuscript received 5 Feb 85) Vol 23, No 12, Dec 87  
pp 1594-1605

[Article by V.A. Butenko, B.G. Grishlenkov, A.M. Arkharov, A.V. Vitkovskiy, and A.S. Gastev, Moscow Higher Technical School imeni N.E. Bauman, Institute of Medical and Biological Problems, Moscow]

[Abstract] A study of processes of heat and mass exchange in an electrochemical system for removing carbon dioxide from an atmosphere with simultaneous regeneration of oxygen from water under nonstationary and nonisothermal conditions was described and discussed. The system consists of closely packed porous electrodes, between which there is a porous absorber, separated from the anodic and cathodic electrodes by a diaphragm filled with a concentrated solution of KOH + K<sub>2</sub>CO<sub>3</sub>. The anode serves as a desorber. The inter-electrode space was studied. Calculations revealed elements in which maximum operating conditions occur. Settling of the electrolyte into the precipitate may occur in the absorber, where the bicarbonate concentration reaches the maximum level, and in the desorber-anode, where the carbonate concentration is maximal. The maximum current in the system may be achieved from the back side of the desorber-anode, where the hydroxyl ion concentration may drop to zero. There was good conformity between the values of the theoretical and experimental coefficients of electrochemical absorption, which confirmed the effectiveness of the absorption process in the electrochemical system. Figures 7; references 6 (Russian).

02791

**Cathode Reduction of Fluorinated Glass Carbon**

18410203b Moscow *ELEKTROKHIMIYA* in Russian  
(manuscript received 1 Aug 86) Vol 23, No 12, Dec 87  
pp 1648-1652

[Article by Ye.M. Shembel, O.S. Ksenzhek, Ye.A. Vasileva, A.S. Fialkov, and V.S. Dubasova, Dnepropetrovsk Chemical Engineering Institute imeni F.E. Dzerzhinskii, All-Union Institute of Electrical Carbon Products, Elektroglu]

[Abstract] Fluorinated carbon is a promising solid-phase active cathode material for lithium high power capacity batteries. The advantages of a lithium-carbon system in

comparison with other lithium batteries include its high specific characteristics, flat discharge curve, and good shelf life even at a high temperature. This article described a study of polarization properties of fluorinated glass carbon in electrolytes based on solvents with different solvating capacities. The process of reducing fluorinated glass carbon was presented schematically in terms of sequential stages: diffusion in the electrolyte of solvated lithium cations toward the electrode surface; desolvation of lithium cations; reduction of the fluorinated glass carbon, accompanied by the formation of free fluorine bonds and the introduction of desolvated lithium cations; and formation of intermediate reduction products. This may be followed by two parallel processes. The first is the solid-phase dissociation of the intermediate reduction product at the electrode/electrolyte interface, which is determined by interaction of solvent molecules found in the electrolyte and the lithium cations found in the solid phase under the influence of the concentration gradient and the electric field deep in the solid phase. The second of the two processes is accompanied by a corresponding shift in electron density of the bond between the fluorine and carbon toward the electrode/electrolyte interface. Figures 3; references 8: 3 Russian; 5 Western

02791

**Electrode, Light-Sensitive Materials R and D at Electrochemistry Institute**

18410338c Moscow *VECHERNYAYA MOSKVA* in Russian 23 Mar 88 p 2

[Excerpt] Highly active electrodes for chemical sources of current, instruments for monitoring the environment, silver-free composite materials that are sensitive to light, and many other developments of personnel at the Institute of Electrochemistry imeni Frumkin, USSR Academy of Sciences, can be utilized broadly in the economy.

"The new conditions of business management affect Academy institutes to a certain extent," said Professor V. Kazarinov, director of this institute. "Now we must not only engage in basic research, but also promote introduction of our developments into practice as quickly as possible."

The institute also maintains broad international ties with academies of sciences of socialist countries; it is taking part in projects in line with the program "Elektrokhimiya" [electrochemistry] as well as in the Comprehensive Program of Scientific-Technical Progress of CEMA member-countries.

**Chemical Warfare Specialist Shares Experience  
Gained at Chernobyl**

18410338a Moscow KRASNAYA ZVEZDA in Russian  
29 Apr 88 p 2

[Article by General-Lieutenant A. Kuntsevich, Academician, deputy head of Chemical Troops of the USSR Ministry of Defense, and Hero of Socialist Labor]

[Abstract] The author recalls emergency operations in which he and other representatives of the armed forces took part, following the accident at the Chernobyl Nuclear Power Station. As a specialist in chemistry, he mentions that chemical materials played an important part in decontamination work at this station, and he notes the military importance of synthetic materials.

The author relates that a strategy for eliminating consequences of the Chernobyl accident over an extensive area was drafted with the participation of leading organizations of the USSR Academy of Sciences, a State commission for preparing basic recommendations, regarding decontamination methods, and representatives of the USSR Ministry of Defense and other government agencies. All assignments were drafted and

approved in only three days. At the station, a small contingent of chemical and engineering troops began the first stage of decontamination in conditions of high levels of radiation in certain places, continuous escape of radioactivity into the atmosphere, uncertainty about the physical state of the damaged reactor, and lack of experience with work in such conditions. Successful completion of this stage made it possible to increase the number of personnel involved in the emergency operations and begin decontamination work both on the territory of the station and inside it. With the return of conditions to normal in the accident zone, the author expects participation of servicemen in the cleanup to decrease.

On the basis of experience obtained at Chernobyl and results of psycho-physiological studies, the author mentions traits which he feels should be possessed by personnel taking part in operations in extreme conditions, such as those created by modern chemical and nuclear weapons. These traits include maximum preparedness to fight and work in such conditions, strong will, and emotional stability. Commanders and engineers should possess not only technical erudition, but also the ability to analyze diverse information efficiently and to solve problems jointly with their colleagues.

**Physicochemical Study of Triple Oxides, Formed in Systems AO- $\text{Ln}_2\text{O}_3\text{-SnO}_2$  (A = Mg, Ca, Zn)**  
18410194b Moscow *ZHURNAL NEORGANICHESKOY KHMII* in Russian Vol 32, No 12, Dec 87 (manuscript received 12 Jul 85) pp 2887-2890

[Article by O.V. Godzhiyeva, N.V. Porotnikov, and N.A. Korobkina]

**[Abstract]** Recently, much attention has been devoted to studying the physical chemistry of oxide systems of the type AO- $\text{Ln}_2\text{O}_3\text{-TiO}_2$ , where A = Mg, Ca, Sr, Ba, Zn; Ln = La-Lu, Y. New triple oxides and solid solutions of these systems that have been synthesized have found broad applications. Literature data on the study of reactions of oxides of the type AO,  $\text{Ln}_2\text{O}_3$ , and stannic dioxide are very limited. A compound having the composition  $\text{MgLa}_2\text{SnO}_6$ , which crystallizes into the perovskite structure, is known to exist; however, its crystallographic and electrophysical characteristics have not been determined. In the present work, a systematic study was made of reactions in the aforementioned triple oxide systems where A = Mg, Ca, Sr, Ba, Zn in the sub-solidus region. Triple oxides having the composition  $\text{A}_2\text{Ln}_2\text{SnO}_7$ , where A = Mg, Ca, and Ln = La-Nd, and the compound  $\text{La}_2\text{Zn}_2\text{SnO}_7$  have high specific resistance and dielectric permeability values with almost zero values for the temperature coefficient of dielectric permeability. This combination of a near-zero temperature coefficient of dielectric permeability and high specific resistance and dielectric permeability values makes it possible to use these compounds as dielectrics. Figure 1, references 7: 5 Russian, 2 Western.

12765

**Physicochemical Study of Compounds Based on Zinc, Titanium, and Rare Earth Element Oxides**  
18410194a Moscow *ZHURNAL NEORGANICHESKOY KHMII* in Russian Vol 32, No 12, Dec 87 (manuscript received 12 Jul 85) pp 2884-2886

[Article by O.V. Godzhiyeva, N.V. Porotnikov, and K.I. Petrov]

**[Abstract]** The literature contains references to a study of the triple oxide system  $\text{MgO-R}_2\text{O}_3\text{-TiO}_2$ , in which the existence of compounds  $\text{R}_2\text{MgTiO}_6$  (where R = Pr-Er, Y) has been established. The aforementioned triple oxides have a structure derived from perovskites with varying distortions. The systems  $\text{ZnO-R}_2\text{O}_3\text{-TiO}_2$  have not been thoroughly studied. Evidence of the isolation of individual compounds ( $\text{La}_2\text{MgTiO}_6$ ,  $\text{La}_6\text{MgTi}_4\text{O}_{15}$ , and  $\text{La}_3\text{Mg}_2\text{Ti}_3\text{O}_{15}$ ), which have the same structures as the corresponding magnesium phases, does exist, however. In the present work, reactions in the oxide systems  $\text{ZnO-R}_2\text{O}_3\text{-TiO}_2$  were studied for the purpose of synthesizing complex oxides that appear promising for use as dielectric materials. Ten triple oxides with a perovskite

structure were synthesized, and their electrophysical properties were determined. The newly synthesized oxides and the previously known  $\text{La}_2\text{TiZnO}_6$ ,  $\text{La}_3\text{Ti}_3\text{ZnO}_9$ , and  $\text{La}_6\text{Ti}_4\text{ZnO}_{15}$  are dielectric substances having negative temperature coefficients of resistance and high values of specific resistivity and dielectric permeability. The electrophysical parameters of the oxides and compositions based on them make it possible to use them as dielectrics in condensers in temperature compensation groups. References 4: 2 Russian, 2 Western.

12765

**New Class of Glasses for Integrated Optics**  
18410210c Moscow *DOKLADY AKADEMII NAUK SSSR* in Russian Vol 298, No 2, Jan 88 (manuscript received 12 May 87) pp 418-421

[Article by L.B. Glebov, S.K. Yevstropyev, N.V. Nikonorov, USSR Academy of Sciences Corresponding Member G.T. Petrovskiy, and O.S. Shchavelev, State Optical Institute imeni S.I. Vavilov, Leningrad]

**[Abstract]** Glass is one of the most promising materials for making integrated optical components, and ion exchange diffusion from molten salts is one of the more widely used methods for making glass wave guides. The most essential properties characterizing optical wave guides are refractive index increment, thickness of the light-transmitting layer, and birefringence. Recently, much work has been done to broaden the range of properties for different design problems. The optical properties of waveguide layers depend greatly on the type of ion-diffusate. Although silver ion, one of the most widely used, does increase the refractive index and thickness of the light transmitting layer, its use is limited, due to high light extinction and low thermal and chemical resistance. The refractive index may also be increased by using tellurium ion, although its high toxicity also limits its use for mass production of waveguides. Thus, in order to develop waveguides having the required parameters for integrated optics, it has become necessary to develop new specialty glasses. In the present work, an attempt was made to develop a new class of waveguides having widely varying properties. It has been demonstrated that refractive index increment, birefringence, and waveguide thickness during low-temperature ion exchange are determined by the compression stresses acting within the ion exchange layer and that the magnitude of these stresses is determined by the difference between rates of mass transfer stress relaxation and is a function of the chemical composition of the glass and the process temperature. Controlled alteration of the ratio of these rates may be used as the basis for a new approach to creating wave guides having preassigned properties. The rate of stress relaxation is known to increase markedly as the glass transition temperature is approached. Thus, by using glasses having high glass transition temperatures, it is possible to increase the ion exchange temperature and thereby obtain high compression

stresses, which in turn results in an increased refractive index and birefringence. In the present work, a specially prepared sodium zircon silicate glass having a glass transition temperature of 770° C and an industrial sodium borosilicate glass (glass transition temperature, 560° C) were used. The samples were treated in molten potassium nitrate at 350-560° C for 0.1 to 10 hours. Waveguide parameters were measured by resonance excitation of waveguide modes. Waveguides prepared from sodium zircon silicate glass have radiation losses comparable to that of the sodium borosilicate. Curves showing the effective increment in the refractive index of waveguide modes plotted against diffusion time intersect. This effect may be used to generate higher harmonics, and the high birefringence value may be used to make effective waveguide mode selectors, while the great thickness of the light-carrying layer may be used to join flat and curved waveguides. Thus, waveguides fabricated from sodium zircon silicate glasses may be promising materials for developing various planar integrated optical devices. Figures 3; references 12: 10 Russian, 2 Western.

12765

#### Electroadhesive Method for Joining Superconductors

18410338d Moscow MOSKOVSKAYA PRAVDA in Russian 13 Apr 88 p 3

[Article by V. Mikhaylova]

[Excerpt] How to join two superconductors to each other or join superconductors to other kinds of materials? Welding is difficult and takes much time. What about superconducting adhesives? Yes, this is one solution. But there is still another and simpler way, which has been proposed by Yu.M. Yevdokimov, docent of the Chair of Chemistry at the Moscow Forestry Engineering Institute.

"It is a question of bonding solids without the aid of adhesives," related Yevdokimov. "The method of bonding is the so-called electroadhesive one. An electric field plays the role of adhesive in this case. High-temperature superconductors can be bonded in fractions of a second by means of very thin dielectric films without applying pressure. This can be accomplished both at room temperature and at cryogenic temperatures as low as the temperature of liquid helium."

The method is also suitable for joining solids at high temperatures (up to several hundred degrees). Associates of the Forestry Engineering Institute have succeeded in obtaining just such bonds, whose strength has proved to be fairly high.

Initial results provide good reason for continuing research in the direction that has begun, in the scientists' opinion.

#### Superconducting Polycrystals Developed at Single-Crystals Institute

18410338e Moscow PRAVDA in Russian 30 Apr 88 p 3

[Text] Kharkov, 29 Apr (TASS) — Currents with densities as great as 1,000 A/cm<sup>2</sup> of conductor section can be transmitted through polycrystals which scientists at the All-Union Scientific Research Institute of Single Crystals have developed. Moreover, these new materials are many times as strong as ordinary superconducting ceramics, which are distinguished by heightened brittleness and a porous structure.

This is a step toward solving a problem which physicists of all countries have faced since high-temperature superconductivity was discovered — developing materials which withstand high-power currents.

The Kharkov scientists have already developed a collection of dozens of high-temperature superconductors. They are trying to increase their capability to conduct currents with still greater densities as well as to impart the necessary plasticity to these materials, since cables, assemblies of cryogenic machinery, and other products will probably have to be produced from them.

#### High-Temperature Superconductivity Research at Leningrad State University

18410338f Leningrad LENINGRADSKAYA PRAVDA in Russian 17 Apr 88 p 2

[Article by S. Samoylis]

[Excerpt] Studies of the "greatest scientific discovery of this century" are in progress at the Scientific Research Institute of Physics at Leningrad State University (LGU). This is what high-temperature superconductivity is now being called, and rightfully so.

"At our institute, Ye.F. Gross, corresponding member of the USSR Academy of Sciences, has made a discovery connected with the mechanism of this most interesting phenomenon," said N.V. Borisov, deputy director of the Physics Institute in charge of science. "Much experience with studying the complex substances that superconductors are has also been amassed at LGU. A large-scale program has been drawn up on the basis of our scientific erudition. The Scientific Research Institutes of Physics, Chemistry, and Geology and appropriate schools of the University are now working in line with this program."

M.V. Belousov, senior science associate of the University's Department of Solid-State Physics, is working in close contact with scientists of the Engineering Physics Institute, USSR Academy of Sciences. Among the partners of LGU are the Academy's Institutes of Nuclear Physics, Silicate Chemistry, and other institutes.

Doctor of Physical-Mathematical Sciences, Professor B.V. Novikov, told me that this research already makes it possible to look into the future not only of the "miracle of the 20th Century," but also of physics as a whole.

[A photograph is given, showing M. Belousov working with optical equipment.]

**Synthesis, Structure, and Optical Properties of NdPS<sub>4</sub>**

18410194c Moscow ZHURNAL

NEORGANICHESKOY KHIMII in Russian Vol 32, No 12, Dec 87 (manuscript received 11 Jul 86) pp 2899-2901

[Article by A.N. Volodina, T.B. Kuvshchinova, S.I. Maksimova, E.N. Muravyev, Sh.A. Niyazov, V.P. Orlovskiy, K.K. Palkina, and N.T. Chibiskova, Institute of General and Inorganic Chemistry imeni N.S. Kurnakov, USSR Academy of Sciences]

[Abstract] This work is a continuation of a study of the structure and properties of rare earth element tetrathiomonophosphates having the composition LnPS<sub>4</sub>. Stoichiometric quantities of phosphorus pentasulfide and neodymium sesquisulfide were kept at a temperature of 700° C and a pressure of 0.133 Pa for 65 hours to synthesize the title compound in a fine crystalline state. Increasing the heating time and cooling the compound gradually resulted in the formation of fine (1-2 mm) needlelike single crystals having a pale lilac color. X-ray analysis revealed that the structure of these crystals is based on isolated distorted PS<sub>4</sub> tetrahedra and Nd<sub>3</sub> polyhedra in the form of distorted tetragonal antiprisms bound to one another with common edges and corners. Luminescent spectral analysis indicates that the closest surroundings of the Nd<sup>3+</sup> ion in LaPS<sub>4</sub> have a tetragonal symmetry (the luminescent spectra of this ion in the matrix resemble the spectra of this same ion in YPO<sub>4</sub>). An anomalous long-wave shift (about 15 nm) was observed in the transitions of the Nd<sup>3+</sup> ion in LaPS<sub>4</sub> that has not been observed previously in any of the known spectra of inorganic compounds that have been activated by this ion. Figures 2; references 5: 3 Russian, 2 Western.

12765

**Photo-Quenching and Relaxation Reduction of Excimer Fluorescence of Naphthalene in Polymethyl Methacrylate**

18410261c Moscow IZVESTIYA AKADEMII NAUK SSSR. SERIYA KHIMICHESKAYA in Russian No 1, Jan 88 (manuscript received 1 Jul 87) pp 196

[Article by A.V. Kutsenova and V.M. Anisimov, Institute of Chemical Physics, USSR Academy of Sciences, Moscow]

[Abstract] An anomalously rapid reduction in the intensity of the excimer fluorescence of naphthalene in polymethyl methacrylate was detected. The substance was irradiated with UV light in the long-wave band of absorption of the additive ( $\lambda$  is greater than 290 nm). The quantum yield of photo-quenching of the excimer fluorescence, assuming that a pair of the additive's molecules occupies the position necessary for formation of the excimer until a quantum of light has been absorbed, and assuming that the absorption coefficient does not change, is on the order of one, whereas the quantum yield of the photochemical breakdown of naphthalene under similar conditions is 0.0009 in air and 0.009 in helium. The results indicate that light activity changes the distribution of molecules from the standpoint of the probability of the formation of excimers. Acceleration of the relaxation processes in the medium leads to some restoration of the initial distribution. In this respect, the restoration kinetics of the intensity of excimer fluorescence may characterize the relaxation processes in a medium and thus provide a method of studying the latter. References 4: 2 Russian, 2 Western.

06508

**Crystalline and Molecular Structure of 1-tert-Butoxysilatrane**

18410144 Moscow *DOKLADY AKADEMII NAUK SSSR* in Russian Vol 297, No 5, Dec 87 (manuscript received 30 Sep 86) pp 1123-1125

[Article by A.A. Macharashvili, V.Ye. Shklover, Yu.T. Struchkov, V.P. Baryshok, Corresponding Member, USSR Academy of Sciences, and M.G. Voronkov; Institute of Elemental Organic Compounds imeni A.N. Nesmeyanov, USSR Academy of Sciences, Moscow]

[Abstract] The silatrane  $XSi(OCH_2CH_2)_3N$  have unusual stereoelectronic structure, specific reactivity, and biological activity. For example, 1-alkoxysilatrane ( $X-AlkO$ ) have antitumor, wound-healing, hypolipidemic, and pilotropic action, and they increase the productivity of the Chinese silkworm (*Bombyx mori* L.). The authors of this article undertook an X-ray structural investigation of 1-tert-butoxysilatrane to obtain precise values of its molecular parameters. The colorless crystals were rhombic:  $a = 19.11(2)$ ,  $b = 6.551(7)$ ,  $c = 9.654(7)$  Angstroms,  $V = 1,209(2)$  Angstroms $^3$ ,  $d_{calc} = 1.360$  g cm $^{-3}$ ,  $Z = 4$   $C_{10}H_{21}NO_4Si$ , spatial group  $Pna2_1$ . The lattice parameters and intensity of 1,870 independent reflections were measured at -120° C. The crystal's structure was interpreted by the direct method and was refined by using the least-squares method in an anisotropic approximation for nonhydrogen atoms. The atoms' coordinates and thermal parameters were depicted, as were the molecule's geometry and bond lengths. References 15: 13 Russian, 11 Western.

06508

**Chelated Cobalt Complexes as Catalysts for Oxidative Cleavage of DNA Chains**

18410210a Moscow *DOKLADY AKADEMII NAUK SSSR* in Russian Vol 298, No 2, Jan 88 (manuscript received 8 May 87) pp 363-366

[Article by USSR Academy of Sciences Corresponding Member M.Ye. Volpin, Academician D.G. Knorre, G.N. Novodarova, M.Yu. Tuvn, O.S. Fedorova, and Ye.I. Frolova, Institute of Elemental Organic Compounds imeni A.N. Nesmeyanov, USSR Academy of Sciences, Moscow; Novosibirsk Institute of Bioorganic Chemistry, Siberian Department, USSR Academy of Sciences]

[Abstract] Interest in studying interactions of DNA with transition metal complexes is due to the wide-scale search for anti-tumor preparations and new approaches for selectively modifying nucleic acid structures. Attempts have been made to develop nucleotide derivatives based on specific reagents capable of directed or "addressed" interaction with some predetermined portion of the DNA chain. More recently, it has been observed that iron and copper complexes, while catalyzing the formation of oxygen groups (hydroxyl, peroxide) in the presence of oxygen and a reducing agent, are also capable of cleaving the DNA molecule. It has been

hypothesized that these same oxygen groups are responsible for the cleavage of DNA by certain anti-tumor antibiotics, such as bleomycin and Adriamycin, which occurs with the participation of iron ions. It is further hypothesized that chelated cobalt complexes, being effective catalysts for the oxidation of organic substrates with oxygen, will also cleave DNA chains, i.e., manifest nucleic acid activity. In the present work, an attempt was made to experimentally verify the possibility of cleaving DNA with a catalytically active chelated cobalt complex in the presence of molecular oxygen and a reducing agent. Cobalt complexes with corrin, phen (o-phenanthroline), and salen ( $N,N'$ -bis(salicylidene)ethylene diamine) were prepared and reacted with plasmid pBR322 (DNA target) in the presence of molecular oxygen and ascorbate or hydroquinone as a reducing agent and 0.01 M tris-HCl as a buffer. The reaction was conducted for one hour at 37° C. The results show that the various chelated complexes are capable of catalytically auto-oxidizing an organic substrate and induce effective cleavage of the DNA chain in the presence of a reducing agent and molecular oxygen. These compounds also appear promising in the development of specific reagents for directed action on DNA. References 14: 3 Russian, 11 Western.

12765

**Synthesis and Investigation of Nonamethyl Ferrocenyl Arylcarbinols and Their Cations by PMR Method**

18410261b Moscow *IZVESTIYA AKADEMII NAUK SSSR: SERIYA Khimicheskaya* in Russian No 1, Jan 88 (manuscript received 16 Jul 86) pp 170-175

[Article by A.Z. Kreyndlin, S.S. Fadeyeva, P.V. Petrovskiy, and M.I. Rybinskaya, Institute of Elemental Organic Compounds imeni A.N. Nesmeyanov, USSR Academy of Sciences, Moscow]

[Abstract] The authors previously demonstrated that nonamethyl diferrocenyl carbinol in an acid medium forms diamagnetic nonamethyl ferrocenyl carbenium salts (Ia), where  $R = H$ , which in turn form paramagnetic 1,2-bis(nonamethyl ferrocenium)ethane salts (II), where  $R = H$ , both in solution and in the solid phase. In accordance with the suggested mechanism, it is assumed that the transition (Ia) to (II) occurs through an intermediate cation biradical (Ib) in equilibrium with (Ia). It was assumed that the  $\alpha$ -aryl substituents at the carbenium center sterically hinder duplication of the cation biradical. With this purpose, the authors synthesized arylnonamethyl ferrocenyl carbinols and studied their NMR spectra in both neutral and acidic media. The data obtained indicated that the reduction in stabilization of the carbocation center, resulting from the addition of electron-acceptor groups, leads to an increase in the population of the triplet state, i.e., an increase in the

content of paramagnetic particles. This is the first experimental confirmation of the presence of an equilibrium singlet-triplet transition for ferrocenyl carbenium ions. References 12: 6 Russian, 6 Western.

06508

**Binuclear and Mononuclear Oxygenated Tetraazamacrocyclic Cobalt Complexes**  
18410259a Moscow *DOKLADY AKADEMII NAUK SSSR* in Russian Vol 299, No 2, Mar 88 (manuscript received 26 Jul 87) pp 378-382

[Article by K.B. Yatsimirskiy, academician, Ukrainian Academy of Sciences, Yu.I. Bratushko, A.B. Kondratyuk, B. Yezhovska-Tshebyatovska, A. Vogt, and P. Zhmelevskiy, Institute of Physical Chemistry imeni L.B. Pisarzhevskiy, Ukrainian Academy of Sciences, Kiev; Institute of Chemistry, Wroclaw University, Poland]

[Abstract] The purpose of this work was to synthesize and study the structure and properties of new binuclear oxygenated complexes of cobalt with

5,7,7,12,14,14-hexamethyl-1,4,8,11-tetraazacyclotetradeca-4,11-diene (HTD), containing axial ligands OH<sup>-</sup>, NH<sub>3</sub><sup>+</sup>, ON-C(CN)<sub>2</sub><sup>-</sup>, and NCS<sup>-</sup>, and to produce the corresponding mononuclear complexes which reversibly bond to O<sub>2</sub> in a DMF solution. Compounds with these tetraazamacrocyclic ligands, which are simple models of natural oxygen transporters, were synthesized for the first time. The binuclear oxygenated complexes were isolated in the solid state by crystallization from oxygenated aqueous or aqueous-ethanol solutions. The structure of the complexes and their physical and chemical characteristics were determined by magnetic chemical, EPR, and thermal analysis methods, electron spectroscopy in the 5000-50000 cm<sup>-1</sup> range, and IR spectroscopy in the 100-4000 cm<sup>-1</sup> range. It was demonstrated that dissolving the new binuclear oxygenated complexes of cobalt with HTD in DMF results in the formation of the corresponding mononuclear coordinates and compounds with reversibly bonded oxygen molecules. Figure 1, references 12: 2 Russian, 10 Western.

06508

**Phosphorylated Adamantanes. Part 7.**  
**Functionally Substituted Adamantyl Phosphines.**  
18410260a Leningrad ZHURNAL OБSHCHEY  
KHIMII in Russian Vol 58, No 1, Jan 88 (manuscript  
received 5 Nov 86) pp 33-35

[Article by R.I. Yurchenko, Ye.E. Lavrova, and A.G. Yurchenko, Institute of Organic Chemistry, Ukrainian Academy of Sciences, Kiev]

[Abstract] Reduction of adamantyl dichlorophosphinates with lithium aluminohydride was used to synthesize the first representatives of functionally substituted adamantyl phosphines. The structure of the products was verified by IR and  $^{31}\text{P}$  NMR spectroscopy as well as by conversion to the corresponding carbamates. The presence of other functional groups in addition to the  $\text{PH}_2$  group allows significant expansion of the range of compounds synthesized on the basis of adamantyl phosphines. References 5: 4 Russian, 1 Western.

06508

**Reaction of Phosphorus Pentachloride Adducts and Isoprene with Arsenic Trifluoride**  
18410260b Leningrad ZHURNAL OБSHCHEY  
KHIMII in Russian Vol 58, No 1, Jan 88 (manuscript  
received 5 Nov 86) pp 41-46

[Article by S.V. Gridland and M.N. Miftakhov, Kazan Chemical Engineering Institute imeni S.M. Kirov]

[Abstract] In order to produce fluorine-containing phosphonic acids, the authors studied the reaction of  $\text{PCl}_5$  adducts and isoprene with arsenic trichloride in benzene. The major product was 1,1-dimethylindane, whose structure was confirmed by  $^1\text{H}$  and  $^{13}\text{C}$  NMR and IR spectroscopy. With cyclic derivatives, arsenic trifluoride was incapable of breaking the P-C bond. As was expected, when the reaction was performed without  $\text{PCl}_5$ , there was an exchange of halogens at the phosphorus atom that resulted in the formation of unstable 1,1,1-trifluoro-3-methyl-2-phospholene. It was in turn rapidly converted to relatively stable 1-fluoro-3-methyl-1-oxo-2-phospholene. The reaction of the acyclic adduct of isoprene (or 4-chloro-2-methyl-2-butene dichlorophosphine) and phosphorus pentachloride with arsenic trifluoride in benzene is thus accompanied by its arylation and leads to the formation of 1,1-dimethylindane as the major product. The reaction of the cyclic adduct of  $\text{PCl}_5$  and 1,1,1-trichloro-3-methyl-2-phospholene with arsenic trifluoride yields 3-methyl-1,1-difluorocyclopent-2-ene-1-phosphonium hexafluorophosphate without the formation of arylated compounds. References 16: 7 Russian, 9 Western.

06508

**Reaction of Indoles With Polyfluorocarbonyl Compounds**

18410145a Riga KHIMIYA  
GETEROTSIKLICHESKIKH SOYEDINENIY in Russian No 9, Sep 87 (manuscript received 20 May 86) pp 1200-1201

[Article by A.Ye. Zelenin, deceased, N.D. Chkanikov, Yu.N. Ivanchenko, V.D. Tkachev, V.A. Rusakova, A.F. Kolomiets, and A.V. Fokin, Institute of Elemental Organic Compounds imeni A.N. Nesmeyanov, USSR Academy of Sciences, Moscow]

[Abstract] Indoles react with hexafluoroacetone and methyl trifluoropyrrolacemic acid to form 3-alkylation products that have fungicidal effects on plants. The presence of a substituent at position 2 of the indole does not significantly influence the direction or optimal conditions of C-alkylation reactions of indoles with polyfluorocarbonyl compounds. According to patent data, indole derivatives, containing alkyl and aryl substituents in positions 2 and 3, have a broad spectrum of fungicidal activity. Test results have shown that all of the compounds studied have clear fungicidal activity for brown rust and powdery mildew of wheat. The most active compounds in these tests were the IIIb and Va,b compounds. They achieved a 70 to 90 percent suppression; however, their activity was not equal to that of the commercial fungicide Benlate. References 4: 2 Russian, 2 Western.

06508

**Cleaning Wastewater from Sodium Trifluoracetate Production**

18410145b Kiev KHIMIYA I TEKHOLOGIYA VODY in Russian Vol 9, No 5, Sep-Oct 87 pp 440-441

[Article by T.Yan-V. Boyko, T.M. Levchenko, N.A. Klimenko, and S.I. Vukolova]

[Abstract] World production and consumption of the herbicide sodium trichloracetate exceeds 100,000 tons per year and is expected to continue increasing. Trichloroacetic acid is the most toxic component of wastewater from sodium trichloracetate production. At present, the adsorption method is virtually the only suitable method of cleaning trichloroacetic acid from this wastewater. The biologic method is unsuitable because trichloroacetic acid contaminates activated sludge. Extracting trichloroacetic acid by using organic solvents is ineffective, due to the low distribution coefficient of trichloroacetic acid in the solvents, and using ion exchange with anionites is impracticable because of the rival effect of the salts found in the wastewater. This article presents data about processes using activated carbon to clean the trichloroacetic acid formed during sodium trichloracetate production from wastewater. Complete suppression of ionization occurred only when the pH was less than one, i.e., in concentrated solutions of mineral acids. The limit adsorption of trichloroacetic

acid attained (when there was complete suppression of ionization) was approximately 1 mmol/g or 16.5 percent of the total carbon, which confirms the feasibility of using adsorption technology to extract trichloroacetic acid. Of course, using activated carbon to clean wastewater is only feasible if the sorbent can be regenerated several times. A method of using sodium hydroxide to regenerate the activated carbon was tried and validated. The complete procedure for removing trichloroacetic acid from wastewater from sodium trichloracetate production, as developed in the experiment described in this article, consists of the following steps: adsorption of trichloroacetic acid by activated carbon, treatment of the carbon with a sodium hydroxide solution, desorption of chloroform by water vapor, separation of the condensate, and recovery of the chloroform.

12794

**New Type of Pyrethroid Insecticides**

18410221a Moscow AGROKHIMIYA in Russian No 12, Dec 87 pp 95-102

[Article by N.N. Melnikov and N.I. Aronova]

[Abstract] DDT and hexachloro cyclohexane have been banned from use in agriculture due to their high persistence and the possibility of their entering the human food chain. Organophosphorus and carbamate insecticides, developed as replacements, must constantly be altered because various plant pests build up a resistance to them. Synthetic pyrethroids have attracted worldwide interest because they are highly toxic to many insect pests, including those that have developed a resistance to organophosphorus pesticides. However, these compounds were found to be highly toxic to fish, and their use became limited. Moreover, synthetic pyrethroids are more expensive than organophosphorus pesticides. It has thus become necessary to continue the search for effective preparations that are harmless from an environmental standpoint and readily decomposable into metabolites that do not harm useful species but still have a high enough toxicity against pests, especially those that are resistant to currently used insecticides. They must also be economical to produce. Synthetic pyrethroids, prepared by modifying natural pyrethroids, are esters, and until recently, it was assumed that their insecticidal activity was related to their ester function. Recently, a new group of compounds having an ether configuration has been discovered to have an insecticidal effect similar to that of pyrethroids and DDT. One member of this group, 2-(4-ethoxyphenyl)-2-methylpropyl-3-phenoxybenzyl ether (MTI-500), is currently used in agriculture under the trade name Trebon. It has many of the aforementioned characteristics. Discovery of the insecticidal and acaricidal properties of the 2-arylethyl phenoxybenzene ethers stimulated the synthesis of a large number of derivatives. Further modification of MTI-500 by substituting an alkylene group for the ether bond led to the development of MTI-800, which has a higher toxicity than MTI-500 but is less toxic to fish (the LD<sub>50</sub>

for carp is 40 mg/l for MTI-500 and only 5 mg/l for MTI-800). These new insecticides are similar to pyrethroids but less toxic to the environment (and to fish). They may thus be used safely near water reservoirs and against aquatic pests. They are simpler to prepare and thus more economical than pyrethroids, and they are active against pests with cross-resistance to pyrethroids. References 28: 5 Russian, 23 Western.

12765

**Delayed Neurotoxicity of Organophosphorus Pesticides**

18410221b Moscow AGROKHIMIYA in Russian No 12, Dec 87 pp 103-124

[Article by G.F. Makhayeva, V.V. Malygin, and I.V. Martynov]

[Abstract] Until recently, toxicologists selecting pesticides for general use have focused their interest on the acute and long-term effects of organophosphorus compounds. More recently, however, they have switched their attention to the so-called delayed neurotoxicity of organophosphorus compounds (ONTFOS), characterized by the development of paresis and paralysis some period of time after exposure to the compound and usually lasting 1 to 3 weeks. This ailment is not related to the anticholinesterase activity of the compound and may be caused by compounds not having high toxicity, i.e., ordinary toxicological testing appears to indicate that it does not present any high toxicity. The present review covers basic topics related to the clinical picture, pathomorphology, and mechanism of initiation of ONTFOS and certain interrelationships between the structure of an organophosphorus compound and its capability of causing a delayed neurotoxicological effect. References 123: 5 Russian, 118 Western.

12765

**Synthesis of N-Alkylbenzoxazoline Thiones**

18 1264c Tashkent UZBEKSKIY KHIMICHESKIY ZHURNAL in Russian No 6, Nov-Dec 87 (manuscript received 6 Jul 87) pp 39-40

[Article by K. Giyasov and N.A. Aliyev, Order of Labor Red Banner Institute of the Chemistry of Plants, Ukrainian Academy of Sciences; Tashkent Order of Friendship of the People Agricultural Institute]

[Abstract] Benzoxazoles and benzothiazoles have a broad spectrum of pesticidal activity. Some of them, such as S-alkylthiobenzothiazoles, have a defoliant effect. To develop a convenient method for synthesis of

N-alkylbenzoxazoline thiones (ABT) and to study their defoliant activity, the authors investigated the isomerization of S-alkylthiobenzoxazoles at 150-220° C in the presence of crystalline iodine, producing N-alkylbenzoxazoline thiones with good yield. The isomerization could not be performed without catalysts. The compounds synthesized were crystalline substances that were easily purified by n-hexane, including some not described in the literature. The S-alkylthiobenzoxazoles and alkylbenzoxazoline thiones synthesized had a moderate defoliant activity on model cotton plants under natural conditions, with S-alkylthiobenzoxazoles having the greater defoliant activity. References 7: 4 Russian, 3 Western.

06508

**Chlorination of o-Di(mercaptomethyl)benzenes and Their Cyclic Disulfides**

18410264b Dushanbe DOKLADY AKADEMII NAUK TADZHIKSKOY SSR in Russian Vol 30, No 6, Jun 87 (manuscript received 17 Feb 87) pp 370-371

[Article by I.S. Salitra, S.V. Zyryanov, I.G. Shanyavskiy, and I.M. Nasirov, Institute of Chemistry imeni V.I. Nikitin, Tadzhik Academy of Sciences]

[Abstract] Cyclic thioacetals have been used as intermediates in the synthesis of pesticides. This article discusses the results of chlorinating 4,5-dimethyl-o-xylene- $\alpha,\alpha'$ -dithiol (I) and 1,4-dihydro-6,7-dimethyl-2,3-benzodithiine (II) in order to produce 4,5-dimethyl-o-xylene- $\alpha,\alpha'$ -disulfenyl chloride, which is subsequently used in a reaction with CH<sub>2</sub>-active carbonyl compounds. Compounds I and II were chlorinated in a medium of dry ethyl acetate at -15 to -20° C in a nitrogen atmosphere. Sulfuryl chloride was added at 2.1 moles per mole of I or 1.05 moles of II and agitated for one hour. Next, the mixture was agitated for an additional 0.5 hour. A solution of the carbonyl compound in ethyl acetate was gradually added over 15 minutes to the reaction mixture, agitated another 30 minutes, and allowed to warm to room temperature. The proposed structure was verified by mass spectroscopy, NMR, and elemental analysis. The proposed chlorination mechanism for the formation of the di(2-chloromethyl-4,5-dimethylbenzyl)disulfide is illustrated. The results obtained make it possible to conclude that when 4,5-dimethyl-o-xylene- $\alpha,\alpha'$ -dithiol and 1,4-dihydro-6,7-dimethyl-2,3-benzodithiine are chlorinated by sulfuryl chloride, di(2-chloromethyl-4,5-dimethylbenzyl) is formed instead of the expected sulfenyl chlorides. References 4: 1 Russian, 3 Western.

06508

**Computer-Assisted Search for Polymers with Preassigned Physical and Chemical Properties**  
18410196b Moscow VYSOKOMOLEKULYARNYYE SOYEDINENIYA in Russian Vol 29, No 11, Nov 87  
(manuscript received 17 Jun 86) pp 2433-2440

[Article by A.A. Askadskiy, Ye.G. Galpern, T.P. Matveyeva, A.L. Chistyakov, and G.L. Slonimskiy, Institute of Elemental Organic Compounds imeni A.N. Nesmeyanov, USSR Academy of Sciences; Moscow Construction Engineering Institute imeni V.V. Kuybyshev]

[Abstract] Much work over the past 10 to 15 years has been devoted to the problem of predicting the physical properties of a polymer from its chemical structure. Two monographs exist that outline the approaches to computing the physical characteristics of a polymer purely from data on the chemical structure of the repeating unit. These approaches are based on the additivity of various atoms and atomic groups in the characteristic being examined. It has now become possible to perform such tasks directly and in reverse on a computer, i.e., to determine one or several physical properties from data on chemical structure or to predict the chemical structure of the repeating unit of that polymer that possesses certain required characteristics of physical properties. In the present work, a BESM-6 computer was used to develop a program for computing the physical and chemical properties of a polymer, based on the chemical structure of its repeating unit. The program also makes it possible to perform the reverse task. Physical property inputs (and their algorithms) include density, glass transition temperature, coefficient of thermal expansion in the glass state, temperature of initiation of intense thermal destruction, glass transition temperature-to-melting point ratio, refraction index, cohesive energy density (Hildibrand's solubility parameter), and the optical stress sensitivity coefficient. Chemical structures and increments for 18 groups are presented. References 10 (Russian).

12765

**Cationites with Chlorinating, Oxidizing, and Bactericidal Properties**  
18410196a Moscow VYSOKOMOLEKULYARNYYE SOYEDINENIYA in Russian Vol 29, No 11, Nov 87  
(manuscript received 29 May 86) pp 2346-2352

[Article by R. Bogochev and E. Kotsiolek-Balyaveyder, Institute of Engineering for the Chemical and Food Industries, Economic Academy imeni Oskar Lange, Wroclaw, Poland]

[Abstract] A major disadvantage of certain currently used nitrogen-containing ion exchange resins is that they are subject to mildew formation when prepared in solutions containing biodegradable components. The purpose of the present work was to prepare and study

hydrogen and sodium forms of cationites having bactericidal properties. The cationites were based on a styrene-divinyl benzene copolymer. Multistage chemical modification of a sulfonate-containing styrene-divinyl benzene copolymer with a macroporous structure was used to prepare a cationite containing N-monochlorosulfamide groups. The chemical structure was confirmed by elemental and functional group analysis as well as IR-spectroscopy. The structure's stability was tested in a dry state and in water, 1 N sulfuric acid, and 1 N sodium hydroxide. Sorption capacity and selectivity were determined for a number of cations, and their chlorinating and oxidizing properties and usefulness in the bromination and iodination of organic compounds were studied. Heavily contaminated river water, after treatment with the cationite, showed a 100-fold reduction in total quantity of bacterial colonies. During the course of disinfection, active chlorine passes from the resin to the water in chloride form. As the active chlorine is consumed, the resin may be regenerated with hypochlorite solutions. Figures 6; references 5 (Western).

12765

**Adamantane-Containing Epoxy Compounds and Polymers Based on Them**  
18410184 Moscow PLASTICHESKIYE MASSY in Russian No 12, Dec 87 pp 35-37

[Article by A.K. Shirayev, I.K. Moiseyev, and V.F. Stroganov]

[Abstract] Introducing an adamantane group into the structure of a polymer improves its service properties by raising its resistance to heat and corrosion. However, references to adamantane-containing epoxy compounds and polymers based on them are limited. Epoxy polymers may be modified by introducing an adamantane group into the epoxy compounds themselves or into their hardening systems. Traditional methods of synthesizing epoxy compounds can also be used to prepare adamantane-containing epoxies. In the present review, these methods are divided into the following three groups: esterification of functional adamantane derivatives with epichlorohydrin, epoxidation of unsaturated adamantane compounds with peracids, and conversion of adamantane ketones into epoxies by Darzhan's reaction or sulfur ilides. Another way of obtaining adamantane-containing epoxy polymers is to use hardening systems into which adamantane-series compounds have been introduced. Epoxy polymers hardened by diamines of the adamantane series have high heat stability and exhibit very little shrinkage. Modifying epoxy composites with functional adamantane derivatives is both feasible and promising. References 25: 9 Russian, 16 Western.

12765

**Current-Conducting Polymer Research at Institute of Chemical Physics**

*18410338b Moscow LENINSKOYE ZNAMYA in Russian 20 Mar 88 p 4*

[Article by O. Yefimov, candidate of chemical sciences, laboratory head at a branch of the Institute of Chemical Physics, USSR Academy of Sciences, Noginsk Rayon]

[Excerpt] Production of products with shapes of any kind from polymers is possible in principle. Examples include flat panels which are installed in walls of motor vehicle bodies, large-capacity coil power sources for certain kinds of instruments, and pellet-shaped power sources for electronic clocks or microcalculators.

Scientists are looking for ways of employing a new class of polymers in electronics, for production of diodes, transistors, integrated circuits, and computer storage components, as well as for the purpose of eliminating static electricity and in chemical sensors — devices which respond sensitively to changes in the composition of their environments and to the appearance of harmful substances in the atmosphere or water.

Research of current-conducting polymers is of very recent origin; it is less than 10 years old. But it undoubtedly has a great future. A branch of the Institute of Chemical Physics, USSR Academy of Sciences, is one of the chief organizations in this field. An intensive search for new conductive polymers and ways of employing them on a broad scale is in progress here.

**Ways of Reducing Radioactive Contamination of Soils and Plants**

18410264a Moscow *KHIMIZATSIYA SELSKOGO KHOZYAYSTVA* in Russian No 2, Feb 88, pp 33-35

[Article by M.A. Kuzmich, candidate of agricultural sciences, All-Russian Scientific Research and Engineering Design Institute for Chemicalization of Agriculture]

[Abstract] This article discusses ways of reducing the contamination of plants when soil has been contaminated by the fission products of uranium-235. After a year or two, most soil radioactivity is caused by strontium-90 and cesium-137. Although there are as yet no effective measures for eliminating radioactive elements from soil, deep plowing can turn the contaminated surface layer of the soil over and significantly reduce the assimilation of radionuclides by plants. This approach is

not effective in sandy loam soils, but isotopes migrate rapidly in these soils to lower layers, thus making it unnecessary. Disk harrowing may improve drainage and encourage migration of radionuclides downward into the soil. Selection of the plant type can also reduce uptake of strontium-90. Potassium carbonate has been found effective in reducing the uptake of cesium-137. The addition of cement powder to soil is an interesting approach. Nitrogen fertilizers may increase the uptake of radioactive isotopes by plants, particularly cesium. Phosphogypsum should be used on neutral soils with a high calcium content to limit the uptake of strontium-90. Various sorbents such as zeolites, glauconites, vermiculite, montmorillonite, bentonite, phlogopite, and other nontraditional substances can increase the absorption of radionuclides by soils. References 4: Russian.

06508

**Fluorine-Containing Amino Acids. Part III.  
alpha-Trifluoromethyl Amino Acids**

18410196c Leningrad ZHURNAL ORGANICHESKOV  
Khimii in Russian Vol 23, No 11, Nov 87 (manuscript  
received 18 Jul 86) pp 2308-2313

[Article by V.A. Soloshonok, I.I. Gerus, Yu.L. Yagupolskiy, and V.P. Kukhar, Organic Chemistry Institute, UkrSSR Academy of Sciences, Kiev]

[Abstract]  $\alpha$ -Trifluoromethyl derivatives of  $\alpha$ -amino acids have not been studied until recently. Similar types of compounds,  $\alpha$ -trifluoromethyl alanine and the polyoxy derivatives of phenylalanine, have been shown to possess high biological activity. In the present work,  $\alpha$ -trifluoromethyl amino acids were synthesized by alkylating previously unknown imines of 3,3,3-trifluoro pyrotartaric acid with organometallic reagents. The imines' reactivity was demonstrated to be a function of the substituent at the nitrogen atom.  $\alpha$ -Trifluoromethyl amino acids are also potential inhibitors of pyridoxal phosphate-containing enzymes and, by analogy with  $\alpha$ -methyl amino acids, appear to be promising as components of physiologically active peptides.  $\alpha$ -trifluoromethyl- $\alpha$ -amino acids synthesized by the new method are being studied from the standpoint of their biological activity. References 9: 3 Russian, 6 Western.

12765

**Evaluating Inventions Based on Discoveries in Chemistry**

18410202b Alma-Ata VESTNIK AKADEMII NAUK  
KAZAKHSSKOV SSR in Russian No 11, Nov 87, pp  
68-73

[Article under the "Effectiveness and Quality of Scientific Research" rubric by G.M. Dzhilkibayeva, G.A. Dyachkov, and V.A. Senchevskaya]

[Text] The modern period of scientific development is distinguished by the complexity of the problems being worked on to hasten scientific-technical progress [1]. The fast pace of development in science and industry demands close contact between scientific-technical and industrial activity. The structure of scientific-technical activity may be conceived as integrated, mutually interconnected studies of fundamental and applied natures, whose results are formulated and collected both in the publication archive, which records the events and the forms of accretion of knowledge, and in the projects implemented on the basis of this knowledge [2].

The publication archive includes the subsystems of the fundamental archive, the archive of applied research, and the archive of patent documentation on inventions and discoveries. Each of the subsystems, and the publication archive as a whole, evolves over time while preserving its stability, since the end product of scientific-technical activity, involving fundamental and applied research is formulated in a standard unified form: from

the scientific article to the survey, the catalog, the State Standard, and the patent documentation on inventions and discoveries. It is the information of the archive of patent documents which is closest to the leading edge of scientific projects in the system of scientific publications gathered in the publication archive. The former assembles data on the exceptionally large scientific-technical potential built up over many years in all the nations of the world. This objectively reflects the dynamism of scientific-technical progress [3].

Discoveries hold a special place in the system of accumulating scientific knowledge, generally being the outcome of scientific-technical activity in the field of fundamental research, but, expressed in a unified, standard form (the specification of the discovery), they gather dust in the archive of patent documents.

The goal of the present article is to identify the interconnections and interrelationships in the discovery-invention system, as well as the influence of discoveries on the interdisciplinary interworking of the scientific disciplines.

The practical effectiveness of a discovery is expressed in terms of the new knowledge which it creates. A discovery can be viewed as a system which includes a complex of interconnected elements: the inventions, created on its basis and reflecting a certain unity. The nature of the discovery is expressed in its formulation, and therefore, the formulation of a discovery may be regarded as a system comprised of subsystems—the inventions. In turn, an invention is treated as a constituent element of a certain higher-order system, the discovery. To solve the stated problem by means of a systematic approach, we select as the subject of investigation a discovery in the field of chemistry [4]. The discovery, whose subject is a "phenomenon," was first registered in 1966 (certificate No 38), the "property" in 1967 (certificate No 51), and the "mechanism" in 1971 (certificate No 101). We explore the correlation in the discovery-invention system by the example of discoveries in the field of polymer and organic chemistry, viewed under three aspects:

temporal changes in the system as a whole;

the link between the system and its environment (the interdisciplinary interaction);

the evolution of the environment in the presence of the system.

To determine the temporal changes of the system, we take as our basis the priority date of the discovery as an objective index, corroborating the advent of new knowledge. The intense development of polymer chemistry made possible five major discoveries in the late sixties. The advent of new knowledge, expressed in the specification of discovery, carries with it the potentiality of creating new technical designs in a more compressed timeframe than if the inventions were to occur in the

Открытия в области химии

Номер охранных документов (a)	Объект открытия (b)	Дата приоритета (c)	Дата поступления заявки на открытие (d)	Основание для установления приоритета (e)	Дата регистрации открытия (f)
38	Явление (g)	10.02.61	03.07.64	Доклад	27.04.66
97	•	12.06.64	15.05.69	(i)	20.04.71
113	•	20.05.68	01.06.71	•	17.04.72
125	•	23.06.64	23.06.64	(f)	19.03.73
167	(h)	26.06.61	27.03.73	•	30.10.75
168	Закономерность (h)	22.04.60	24.10.73	•	20.11.75
184	Явление	11.01.74	30.01.74	•	07.04.77
		30.04.68		•	
188	•	22.12.67	14.04.76	•	22.09.77
		18.02.71		•	
199	•	19.03.68	06.03.75	Доклад	13.04.78
204	•	19.06.65	15.03.76	Статья	21.09.78
205	•	08.01.75	30.12.76	Заявка на открытие (d)	26.10.78
232	•	25.05.63	17.10.75	Статья	26.06.80
248	•	07.10.59	20.07.76	•	06.08.81
		22.02.63		•	

Discoveries in the Field of Chemistry

Key:

- a. Patent document number
- b. Object of discovery
- c. Priority date
- d. Date of submission of declaration of discovery
- e. Basis for establishment of priority
- f. Date of registration of discovery
- g. Phenomenon
- h. Mechanism
- i. Report
- j. Article
- k. Declaration of discovery

absence of the innovation. By the mid-seventies, there was a "burst" of invention applications submitted, largely due to the existence of the new knowledge. From this time onward, the correlation between the discovery and the invention takes a distinct form, and the interaction of the discovery with its environment can be discerned.

It must be noted that the subject of a discovery in the field of organic and polymer chemistry is the phenomenon (cf. table).

The "phenomenon" as a form of manifesting the essence of an object in the material world (nature) should be ranked as the first step in scientific understanding, during which a given scientific achievement is made,

thereby dictating the fundamental importance of the discovery. The next steps in the scientific understanding of the world around us are the "property," a qualitative aspect of the object in the material world, and the "mechanism," a link between "phenomena" and "properties" of the material world. The determination of a previously unknown, objectively existing "phenomenon," "property," or "mechanism," i.e., the advent of new knowledge, enables a new approach in comprehending the nature of chemistry, changes the traditional pattern of thinking, and modernizes the knowledge in the field as a whole. The prospect of a deliberate synthesis of compounds and polymers on a technical level superior to the past is created. This potentiality builds up and manifests itself in new inventions, on the basis of which we move subsequently to a discovery or, conversely, from a discovery to inventions.

As an example, let us consider the discovery of certificate No 188, "The Phenomenon of Existence of a Low-Temperature Limit of the Rate of a Chemical Reaction." It was believed that chemical reactions could not occur close to absolute zero since, according to Arrhenius' law, the rate of chemical reactions declines sharply with lower temperature. However, according to the discovery of certificate No 188, the occurrence of chemical reactions at very low temperatures—near 4.2 K—was demonstrated for the first time. Reactions of polymerization (addition) of crystalline monomers of varying chemical structure were conducted at 4.2 K under conditions where these reactions were initiated by ionizing or ultraviolet radiation. It was also established that reactions at 4.2 K occur at a high rate and with complete conversion of the starting material into the end product, while polymers synthesized at low temperatures are in some cases different in structure from those formed at higher temperatures. On the basis of the discovery, inventions were created that were different in terms of significance from those with a similar purpose. For example, by USSR inventor's certificate No 474540, "A method of producing acetone copolymers," the product yield is 150 times greater than that of the prototype. Moreover, this discovery is bringing new ideas into biology; in particular, it testifies to the feasibility of synthesizing complex organic molecules which constitute the basis of organic matter in conditions of frigid outer space under the action of cosmic rays. We should anticipate the advent of new technical designs in this field of engineering in future.

Using the systems approach to describe the development of science has brought out the synchronicity of its changes as a whole. Inventions are an index of the progressiveness of research, their effectiveness depending on innovation in the particular field of engineering. But discoveries operate on science as a whole and are the determining factor in the appearance of new revolutionary ideas. The invention activity, as well as the patent situation in general, in the field of organic synthesis and polymer chemistry for the period after 1970 bears a pronounced synchronized character over a period of 5-7 years. Analysis of the significance of inventions created at different times reveals that, once an innovation appears, it is then worked out in detail, the methods are improved, and new substances are deliberately synthesized. This process is observed up to the advent of the next innovation, which exerts an influence on the level of knowledge.

A new, previously unknown situation arises, but it is explained as the outcome of accumulating knowledge. A discovery is made, accompanied by new developments—*inventions*. The discovery is generally preceded by patenting of inventions with a substantially greater positive effect than the prototype.

The discovery, as a system, possesses a number of interrelated elements—*inventions*. This system is characterized by orderliness and internal unity, while each

element, and the system as a whole, exhibits autonomous behavior. Analysis of inventions created on the basis of discoveries in the field of organic synthesis and polymer chemistry reveals that it is possible to establish links among the elements of the system: the inventions and the discoveries. The familiar technique of structuring scientific activity in general may be used for the concept "species" as a philosophical category:

genus—general (a certain field of technology);

species—special (a discovery in this field);

element—single (an invention).

The invention-discovery-invention system operates on a dialectical law from the single to the special and from the special to the general or to the single. The improvements which precede the advent of new knowledge fill the gap between the discovery (species) and the invention-prototype (element) in this field:

invention (element) — improvement (modification) — discovery (species) — invention (element)

Harmonic functioning of such "chain" is indeed the essence of modern scientific-technical progress, the end goal of which is the effectiveness of mass production.

The peculiarity of the situation in the case of a scientific discovery in the field of chemistry manifests itself in the fact that its function as a species progressively advances not only toward inventions in a particular field of chemistry, but also creates a new understanding, providing an impetus to the appearance of a new situation in other fields of science, such as biology (certificate No 199). The discovery of certificate No 199 established the phenomenon of thixotropic lowering of internal stresses in polymer systems. It is known that, during production of polymer items (various coatings, films, glue layers, th. ads and fibers), internal stresses arise on account of the imperfect relaxation processes in the articles, resulting in their destruction (peeling, cracking), which reduces the shelf life and operating life. However, as shown by the discovery, if the articles are produced during the stage of thixotropic thickening, such structures will possess drastically reduced internal stress. This phenomenon was noticed in thixotropic systems of various chemical composition, synthesized from oligomers, solutions, dispersions, and melts of polymers. The practical significance of the discovery lies in the fact that ways have been found to lower internal stresses in polymer systems. In addition, the thixotropic state is also characteristic of natural high molecular weight compounds which comprise the structure of cells in living organisms and the intercellular substance, such as proteins, nucleic acids, and polysaccharides. In this connection, the phenomenon of thixotropic lowering of internal stresses in polymer systems is typical of biochemical processes involved in the growth and vital activities of living organisms, especially in the initial stages of development and genesis of the plant world and living organisms. This discovery in polymer chemistry brings a new understanding

into a different field of science, and the resulting interdisciplinary interaction gives rise to a new situation in biology. This interaction can be represented by the scheme:

chemistry leads to biology; discovery (new understanding) leads to a new situation; inventions lead to more inventions.

The evolution of science in the last stage will depend on the effectiveness of how a particular "chain" functions, and new inventions will appear in the field of biology.

The discovery-invention system in the field of organic synthesis enlarges its functions and is responsible for interaction in the overall system of science as a whole, the system itself being an element of the overall structure. The influence between levels of the discoveries made in this case is determined by the scale of the revolution brought about by discoveries in the fund of knowledge, describing the scientific view of the world.

A special feature of discoveries in the field of organic and polymer chemistry manifests itself in the fact that, when ascertained and experimentally corroborated, they have an applied importance in the majority of cases. This field of science is developing in such a way that it seems possible to draw up a tentative estimate of the significance of a discovery and to provide a qualitative appraisal of the degree of fundamental importance of an innovation in respect to its influence on the scientific-technical revolution. The development of the environment in the presence of the discovery-invention system should be progressive in nature, obeying the dialectical law of transition from quantity to quality.

The degree of development of the environment depends on the significance of the system itself, as expressed in the formulation of the discovery and implemented in the inventions. The discovery of certificate No 97, "The Phenomenon of Reaction Coupling on Membrane Catalysts," may serve as an example of the fits and starts in the development of organic chemistry. On the basis of this discovery, the discoverers created around 20 inventions in a brief period, including a full cycle of investigation of the process:

development of a synthesis technology for organic compounds;

development and improvement of palladium-based catalysts;

methods for producing membrane catalysts;

a catalytic reactor for implementing the process.

The practical significance of the given discovery is estimated by the high level of chemical production, much superior to the previous. Quantitatively, such an estimate can be drawn up approximately by analyzing the formulation of the invention, created on the basis of the discovery. The applied importance of the invention is the positive

effect that society will derive from the use of the given invention. The inventions developed on the basis of discoveries are "extraordinary" in that they are intended to modernize existing technology, to boost the product yield, or to be simply "pioneering," with no stipulation section in the patent formulation (USSR inventor's certificate No 870393). The essence of the discovery expounded in the formulation is transferred to the formulation of the invention, while the goal of the invention reflects the rank (level) of the discovery. The strength of influence ( $S_i$ ) of the discovery-invention system on scientific-technical progress (the environment) can be represented by the formula:  $S_i = E_i - E$ , where  $E_i$  is the effect of inventions under the influence of the new knowledge (the discovery) and  $E$  is the possible effect (without the influence of the discovery). The term "environment" in this case includes the new situations (or entire fields of technology) created, the modernization of scientific progress, and the upgrading of the existing industry. The modern stage of development of science is characterized by considerable acceleration, being impulsive and uneven in nature. This factor must be taken into account in the patent research which precedes scientific project developments and influences their effectiveness. It is advisable to include an analysis not only of inventions, but also of discoveries in the particular field of technology in the overall assessment of a patent situation.

Thus, information concerning discoveries involves the latest technical innovations. It furnishes us with knowledge as to the current level and future trends in development of science and technology, activates creative thought, and assists in the search for new solutions. On the basis of discoveries, new directions of development of science are formed, both in the fields of fundamental and applied research. Bibliography 1. Gorbachev, M. S., "Political Report of the Central Committee of the CPSU to the 27th Congress of the Communist Party of the Soviet Union, Politizdat, M., 1986, 127 pp. 2. Mirskiy, E. M., "Mezhdistsiplinarnyye issledovaniya i distsiplinarnaya organizatsiya nauki [Interdisciplinary Studies and the Disciplinary Organization of Science]", Nauka, M., 1980, 280 pp. 3. Afanasyev, V. G., "Man in the World of Systems," NAUKA V SSSR, No 6, 1986, pp 117-126. 4. Dzhilkabayeva, G. M., Senchevskaya, V. A., Dyachkov, G. A., "Systematization of Scientific Discoveries in the Field of Chemistry," VESTNIK AN KAZSSR, No 1, 1987, pp 53-56.

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#### Quantum Chemical Calculations of Spectroscopic Parameters of Heteroaromatic Series Thiones and Selenones and Respective Heterofulvalenes Based on Them

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[Article by A.A. Guliyev, A.Ye. Smolyar, I.A. Abronin, and V.P. Litvinov, Institute of Organic Chemistry imeni N.D. Zelinskiy, USSR Academy of Sciences, Moscow; State Scientific Research Institute of Chemistry and Technology of Elemental Organic Compounds, Moscow]

[Abstract] The increasing interest in the synthesis of organic compounds with high metallic-type electrical-conductivity that has developed in recent years has made it important to obtain quantum chemical data on their physical and chemical characteristics. Experimental studies have shown that at atmospheric pressure as the temperature drops, certain salts based on tetrathiafulvalenes, ion-radical salts, and charge transfer complexes assume a dielectric state that may partially or completely overcome the increase in overlap of the electron wave functions between chains of neighboring molecules, thereby increasing the two- or three-dimensional conductivity related to movement of electrons both along and between chains. Heterofulvalenes that have been condensed with a heteroaromatic ring are promising donor components for such complexes, since the addition of heteroatoms may also vary these phase transitions. This article studies the ionization potentials and electron transition energies of isomer thieno- and selenopheno-1,3-dihetero-2-thiones and -selenones and the heterofulvalenes based on them. Photoelectron and

ultraviolet spectroscopy were performed on several classical donors. The electron transition energies of the thiones and selenones of the heteroaromatic series agreed with UV spectral data. The quantum chemical calculations showed that the asymmetrical isomer thiones and selenones of the heteroaromatic series and their corresponding heterofulvalenes have lower ionization potentials and lower electron transition energies than do their symmetrical isomers and the heterofulvalenes based on them. Increasing the dimensions of the classical donors by annelation with heterocyclic fragments changes the ionization potential and electron transition energy only insignificantly, which is explained by the small contribution of the atomic orbitals of the atoms of these fragments to the outer occupied molecular orbital, the major contribution to the ionization potential being that of the  $4p_{1,3p}$  orbitals of the heteroatoms in positions 2 and 3, as well as the  $2p_{1,3p}$  orbitals of the C atoms which form the double bond. Figure 1, references 14: 3 Russian, 11 Western.

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